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A simple model describing ^3He - ^4He mixtures near a wall

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Résumé. — Nous décrivons l'apparition de l'ordre superfluide au voisinage d'une paroi dans les mélanges ^3He - ^4He par un modèle semi-infini de Blume-Emery-Griffiths. Une analyse du groupe de renormalisation de la version la plus simple de ce modèle conduit à un diagramme de phases qui s'accorde de façon satisfaisante avec les données expérimentales connues.

Abstract. — We describe the superfluid ordering taking place near a wall in ^3He - ^4He mixtures by means of a semi-infinite version of the Blume-Emery-Griffiths model. A renormalization group analysis of the simplest version of this model yields a phase diagram which compares satisfactorily with available experimental data.

The phenomenon of superfluid film formation near a wall in ^3He - ^4He mixtures has been observed for many years [1]. It originates in an effective repulsion of ^3He atoms by the wall. The van der Waals interactions between the wall and ^3He or ^4He atoms are equal, but ^3He atoms occupy a larger volume because of their larger zero-point motion. One observes therefore a higher ^4He concentration near the wall, which may induce a local superfluid ordering [2].

This transition occurs on a line which branches from the λ -line and extends to higher ^3He concentrations, where one eventually observes phase separation near the wall. Figure 1 shows the bulk ^3He - ^4He diagram, with the available data on the location of these transitions. Although various experimental methods have been used to achieve this localization [1], little is known on the details of the transition. In particular, the thickness of the film, the order of the transition, the parameter dependence of the phase diagram have not yet been systematically investigated.

In a previous paper [3] (hereafter referred to as I) we pointed out that the superfluid film formation near the λ -line is analogous to the surface and special transitions in semi-infinite magnetic systems [4]. We described this phenomenon by means of a simple semi-infinite model with short-

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Fig. 1. — Phase diagram for ^3He - ^4He mixtures. Experimental data for surface transitions, taken from Romagnan *et al.* [1], were obtained by several research groups.

range interactions, based on the Blume-Emery-Griffiths [5] (BEG) model for ^3He - ^4He mixtures. We conjectured that the special transition in this model belonged to the same universality class as the « usual », semi-infinite Ising models. Our arguments relied upon a mean-field calculation of the behaviour of the semi-infinite BEG model near the special transition. We also suggested that the same model could be used to describe qualitatively the behaviour of ^3He - ^4He mixtures in the whole range of ^3He concentrations.

In this paper we confirm all the conjectures made in I. The simplest version of the semi-infinite BEG model has been applied to the description of the whole range of ^3He concentrations.

A renormalization group analysis of its behaviour (within the Migdal-Kadanoff approach) has confirmed the stability of the fixed point describing the special transition in the pure Ising model against the perturbation due to a non vanishing concentration of impurities. We have obtained a phase diagram which compares surprisingly well with the existing experimental data.

1. The semi-infinite BEG model.

The BEG model, introduced [5] to describe ^3He - ^4He mixtures, is defined as follows. To each point i of a simple cubic lattice are associated two variables : t_i , σ_i . The variable t_i takes the values 0 (corresponding to the presence of a ^3He atom) or 1 (^4He atom). The variable σ_i takes the values $+1$ or -1 and represents the phase of the ^4He wavefunction. This is a drastic simplification, since one neglects the continuous $U(1)$ symmetry of the superfluid order parameter. This is all the more important in surface phenomena, due to the peculiar nature of superfluid ordering in two dimensions [7] (we will return to this point in the conclusions).

The partition function of the model is given by :

$$Z = \frac{1}{2^N} \sum_{\{t, \sigma\}} e^{-\beta H}, \quad (1)$$

where N is the total number of lattice points, the sum runs over all configurations of the variables t_i , σ_i and

$$-\beta H = - \sum_{\langle ij \rangle} J_{ij} t_i t_j (\sigma_i - \sigma_j)^2 - \sum_{\langle ij \rangle} K_{ij} (t_i - t_j)^2 + \sum_i A_i t_i. \quad (2)$$

The last sum runs over all points in the lattice; the first two ones over all nearest-neighbour pairs. The first term represents the ordering interaction among ^4He atoms; the second describes « isotope » effects (i.e. the difference between the interactions in the ^3He - ^3He and ^4He - ^4He pairs); the parameter Δ plays the role of a chemical potential for ^4He atoms.

This model describes well the observed phase diagram of bulk ^3He - ^4He mixtures already at the mean-field level, yielding superfluid ordering in homogeneous mixtures and phase separation of sufficiently low temperatures [5]. One can straightforwardly extend this model to semi-infinite geometries by taking :

$$J_{ij}, K_{ij} = \begin{cases} J, K & \text{if } i \text{ or } j \text{ belong to the bulk} \\ J_0, K_0 & \text{if } i \text{ and } j \text{ belong to the surface} \end{cases} \quad (3)$$

$$\Delta_i = \begin{cases} \Delta_0 & \text{if } i \text{ belongs to the bulk} \\ \Delta & \text{if } i \text{ belongs to the surface.} \end{cases} \quad (4)$$

Thus, even such a simple model is already described by six parameters. In the absence of more detailed experimental data, which would allow to assign values to some of them, we have preferred to analyse the *simplest* version. We take therefore $K_{ij} = J_{ij}$ which corresponds to the Blume-Capel [8] limit of the BEG model. This amounts to neglecting the differences in the interactions among different isotopes and is quite justified experimentally [5]. We also set $J_0 = J$, supposing no direct effect of the wall on interatomic interactions. We finally take

$$\Delta_0 = \Delta + \phi/kT \quad (5)$$

where the parameter ϕ reflects the phenomenon of effective ^3He repulsion by the wall. As shown in I, the line of onset of film superfluid joins the (bulk) λ -line at a point whose position depends on the value of ϕ . All the data available to us agree in placing this point at a ^3He concentration $x_3 \simeq 0.54$. (This agreement is probably due to the formation of a solid helium layer on the wall of the container, what makes almost irrelevant the composition of the wall.)

2. Renormalization group analysis.

We have performed a real-space renormalization group investigation of this model. The recursion relations which correspond to the doubling of the lattice constant have been derived by Kadanoff's [6] bond moving approach. The one-body interactions have been evenly distributed among the bonds which end at any given lattice point and are then moved along with them [9]. One thus obtains the following recursion relations for the bulk parameters :

$$e^{-4J'} = (e^{-2\tilde{K}} + e^{\tilde{A}-4\tilde{J}})/(e^{-2\tilde{K}} + e^{\tilde{A}-4\tilde{J}} \text{ch } 4\tilde{J}), \quad (6)$$

$$e^{-2K'} = e^{-2\tilde{K}}(1 + e^{\tilde{A}-2\tilde{J}} \text{ch } 2\tilde{J})^2 / [(e^{-2\tilde{K}} + e^{\tilde{A}-4\tilde{J}} \text{ch } 4\tilde{J})(1 + e^{\tilde{A}-2\tilde{K}})], \quad (7)$$

$$e^{4\Delta'} = e^{4\Delta}[(e^{-2\tilde{K}} + e^{\tilde{A}-4\tilde{J}} \text{ch } 4\tilde{J})/(1 + e^{\tilde{A}-2\tilde{K}})]^3, \quad (8)$$

where

$$\tilde{J} = 4J; \quad \tilde{K} = 4K; \quad \tilde{\Delta} = 4\Delta/3. \quad (9)$$

The recursion relations for the surface parameters J_0 , K_0 , Δ_0 have the following expressions :

$$e^{-4J_0} = (e^{-2\tilde{K}_0} + e^{\tilde{\Delta}_0 - 4\tilde{J}_0}) / (e^{-2\tilde{K}_0} + e^{\tilde{\Delta}_0 - 4\tilde{J}_0} \operatorname{ch} 4 \tilde{J}_0), \quad (10)$$

$$e^{-2K_0} = e^{-2\tilde{K}_0} (1 + e^{\tilde{\Delta}_0 - 2\tilde{J}_0} \operatorname{ch} 2 \tilde{J}_0)^2 / (e^{-2\tilde{K}_0} + e^{\tilde{\Delta}_0 - 4\tilde{J}_0} \operatorname{ch} 4 \tilde{J}_0) (1 + e^{\tilde{\Delta}_0 - 2\tilde{K}}) \quad (11)$$

$$e^{\Delta_0} = e^{12\Delta_0/5 + 2\Delta/3} [(e^{-2\tilde{K}_0} + e^{\tilde{\Delta}_0 - 4\tilde{J}} \operatorname{ch} 4 \tilde{J}) / (1 + e^{\tilde{\Delta}_0 - 2\tilde{K}_0})]^2 \times \\ \times [(e^{-2\tilde{K}} + e^{\tilde{\Delta} - 4\tilde{J}} \operatorname{ch} 4 \tilde{J}) / (1 + e^{\tilde{\Delta} - 2\tilde{K}})]^{1/2} \quad (12)$$

where

$$\tilde{J}_0 = 2J_0 + J, \quad \tilde{K}_0 = 2K_0 + K, \quad \tilde{\Delta}_0 = 4\Delta_0/5 + \Delta/3. \quad (13)$$

These recursion relations yield a very complicated flow pattern in the six-dimensional parameter space. (Already for the bulk equations (6)-(9) one has no less than thirteen fixed points [10]). The Blume-Capel limit and the $J_0 = J$ relations are not conserved by the flow. Since we are mainly interested in the phase diagram we use the equations just as a tool for computing the free energy. We iterate them until we reach a fixed point. The nature of the fixed point yields information about the phase we are in. We may thus identify the phase transition lines. The method of Nauenberg and Nienhuis [11] allows us to compute the free energy, and therefore, by numerical derivation, the ^3He concentration x_3 .

Figure 2 shows the results of this computation. The temperature scale is fixed by setting the tricritical temperature at its experimental value. The value of the « rejection parameter » ϕ is chosen in such a way that the special transition takes place at $x_3 \approx 0.54$. The phase diagram we

Fig. 2. — Phase diagram for ^3He - ^4He mixture obtained from the simplest, semi-infinite BEG model. Temperature scale is fixed by the tricritical point temperature ($T_{tr} \approx 0.87$ K). Solid lines correspond to continuous transitions, dotted lines correspond to first order transitions (bulk and surface).

obtain has quite similar features to the experimental one. Two interesting features are not apparent in this diagram :

(a) near the special transition, the surface transition line is curved, according to the results of a scaling analysis (see I, Eq. (7)), however this takes place in an exceedingly small temperature and concentration range ($|\Delta T| \lesssim 0.05$ K);

(b) at concentrations x_3 between 0.85 and 0.95 some changes in the regimes of the stability of the surface fixed points have been observed. This is also the region where the surface phase

transition changes from second to first order. The small value of the surface ^3He concentration in this region makes a detailed analysis difficult. It is possible that in a certain range of temperatures one first observes, in decreasing x_3 , a phase separation with appearance of a film rich in ^4He , but *not superfluid* near the wall. This film then becomes superfluid at a lower value of x_3 . The line of phase separation would end in a critical point. This behaviour would not be surprising, since it appears in a large region of parameter space in the two-dimensional BEG model, as shown e.g. by Berker and Wortis [10].

In fact the Nice experimental group reported in 1978 [1] this possibility of surface phase separation occurring prior to the appearance of superfluidity in the region of high ^3He concentrations. These experiments are rather incomplete and one needs fairly detailed and thorough measurements both of the ^4He concentration and of the superfluid order parameters to verify whether this unusual phenomenon really takes place. We think however that the results of Romagnan *et al.* [1] support our calculations.

3. Discussion.

This investigation was motivated by the need of proving that a simple statistical model is able to describe the essentials of the phenomena observed near a wall in ^3He - ^4He mixtures. We have seen that even a very simple Ising-like model is sufficient, if the semi-infinite geometry is taken into account and the microscopic « rejection effect » near the wall is represented by a single short-range chemical potential term.

In order to obtain a more quantitative description of the phenomena, a more realistic model is needed. The continuous nature of the symmetry broken in the phase transition should be first of all taken into account [12]. This may be obtained by use of the vector generalization of the BEG model [13]. Berker and Nelson have shown that the tricritical point is absent in such a model in two dimensions, and is replaced by a critical endpoint on the phase separation line. One may therefore argue that the phase diagram for the surface transition of the semi-infinite generalized BEG model should present the same topology. This enhances our expectation for the possibility of formation of a normal, ^4He rich, film near the wall in some concentration (temperature range). Moreover, we did not prove that the long-range nature of the wall-mixture interactions is irrelevant for the details of the transitions. It is difficult to investigate this effect by means of the techniques we used, but we do not believe that it seriously affects the picture presented here.

More accurate experimental investigations of the whole phase diagram would be welcome. The determination of the order of the transition and the detailed analysis of the region where the nature of the transition changes are the most urgent questions. Answers to them will determine the direction of further theoretical studies.

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